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**"HALOE Algorithm Improvements for
Upper Tropospheric Sounding"**

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Executive Summary

This report describes our third year efforts to improve the retrieval algorithms used in the analysis of data from the Halogen Occultation Experiment (HALOE) and to extend those results into the upper troposphere. HALOE has continued to function without degradation since its launch in 1991 and has provided a continuous record of middle atmosphere temperature, pressure, O_3, H_2O, NO_2, HF, HCl, NO, CH_4, and multi-wavelength aerosol extinctions during the past decade with a nearly unprecedented precision. This grant has attempted to improve the accuracy of these products and to push the lower limits as far into the troposphere as possible.

Because of its extreme importance, our main thrust has been to use a new signal formulation to permit the retrieval of H_2O in the upper troposphere. This will allow the inference of worldwide tropospheric H_2O trends for the previous 10 years of the HALOE mission and to provide ongoing measurements for the life of the HALOE experiment. This new approach is based on using the HF channel DV/V signal (gas correlated differential signal, DV, divided by the broadband signal, V) that we have previously used for HF retrievals. With the absence of HF in the troposphere and the insensitivity to aerosols and thin clouds, this approach is well suited to retrieve tropospheric H_2O. We have also continued work in a related area, the retrieval of tropospheric CH_4. Since the DV/V methane retrieval goes no lower than about 150 mb due to DV saturation, we have attempted to use other techniques to retrieve CH_4 further down in the atmosphere.

Our analysis of tropospheric clouds, essential for success in the above efforts, has progressed. We have been able to identify for the first time that clouds near the tropical tropopause can be composed of nitric acid trihydrate (NAT) or liquid ternary HNO_3-H_2O-H_2SO_4 aerosols (LTA) [Hervig, 2001]. This work has led directly to improvements in cloud screening algorithms, and has improved our ability to detect and correct cloud contamination.

An unexpected bi-product of our cloud studies is the analysis of HALOE signals at the mesopause and observation for the first time that polar mesospheric clouds (PMCs) are composed of water ice. We have also used our differential water technique to analyze these data and determine the amount of gaseous water that exists in the presence of the PMCs. This has led to improved H_2O and temperature retrievals at mesopause altitudes.

Finally, we have investigated other topics that are potential areas of improvements in the HALOE data set. We have added the latest CH_4 line mixing computations into the operational algorithms. We have investigated the importance of interfering species to determine if we need to update their use in the processing software. We have gone to higher resolution retrievals in the gas correlation channels, increasing our capability to

resolve atmospheric features. Similarly, we have suggested a line-by-line retrieval of O_3 to eliminate band model induced uncertainties below the ozone peak.

The upper troposphere water, improved aerosol for better background models, and resulting low stratosphere upper troposphere methane, would be major additions to upper troposphere/lower stratosphere research. We believe that these, as well as the other improvements described in the first and second year's work, will provide substantial enhancements to an already great data set embodied in the current public release called version 19 (V19). If a version 20 (V20) is produced, the improvements described in this document are essentially completed and ready for use in the operational software.

Background

HALOE is one of the 10 instruments aboard the UARS spacecraft launched in October 1991, and still achieves its original mission objectives with excellent latitude coverage. As a solar occultation instrument, it does not require absolute response calibration, providing results without detectable drift over the duration of the mission. Therefore, it has provided a 10 year data set of the highest quality. The long-term trends of O_3, HCl, HF, H_2O, NO_2, NO, CH_4, multi-channel aerosol extinction, and temperature/pressure have been a major research data source to the scientific community. The HALOE web site at (http://haloedata.larc.nasa.gov/home.html) provides an overview of the spacecraft mission as well as data viewing and access.

The work performed under this three year contract was aimed at improving the quality and accuracy of the data set; extending the altitude range downward into upper troposphere, improving the vertical resolution of the gas correlation channels that produce NO, HCL, HF, and CH_4 retrieval, and adding additional products to the data set. To achieve these improvements we have used unique (to HALOE) signal formulations. For example, to retrieve water in the troposphere we used the DV/V signal from the HF channel.

Overview of Tasks

Our research had nine main objectives, aimed at improving the accuracy of our current products, to obtain new and important products, and to extend the HALOE results into the upper troposphere. Each objective is composed of many smaller and, in some cases, difficult and unexpected tasks. Conversely, they actually comprise a suite of improvements that must to some extent be used together to probe the upper troposphere. We described each of these main objectives in our original proposal. A brief summary follows.

1. *Advanced Pointer-tracker Analysis:* Investigate the possible use of the gimbal angle information in conjunction with ephemeris refraction model data to increase the pointing accuracy in cases of strong atmospheric absorption.

2. *Cloud/Aerosol Identification and Characterization:* Develop a cloud detection algorithm based on the wavelength dependence observed in the HALOE signals, and use this data to create a cloud-top height data set. Improve, modify, and augment as necessary the current aerosol model to extend it into the troposphere, and thus improve the O_3, H_2O, NO_2, and T/P retrievals.

3. *Simultaneous Multi-channel Inversion Algorithm:* Develop a multi-channel retrieval scenario that uses the wavelength dependence of the HALOE measurements coupled with new and existing signal formulations to obtain accurate measurements into the troposphere of H_2O, CH_4, and O_3.

4. *Forward Model Improvements:* Continue to improve the accuracy of forward models through improvements in spectral line lists, band model improvements, and other similar areas. Specific interest should be given to the O_3 and CO_2 (T/P retrieval) models as well as the two continuum models for the O_2 and H_2O absorption that are of particular importance in the H_2O and NO_2 channel retrievals.

5. *Fine Vertical Resolution Gas Cell Retrievals:* Improve the vertical resolution of the gas correlation channel line-by-line retrievals of NO, CH_4, HCl, and HF. In all previous software versions, these retrievals used a 3.0km tangent layer spacing to reduce computational time. By using a grid closer to the radiometer channel retrieval spacing of 0.3km, we will have a more consistent data set. The effective resolution will improve from ~4.0km to ~2.5km.

6. *Improved Pressure Temperature Retrieval:* Use improvements to the CO_2 forward model and the aerosol extinctions from the improved aerosol model to push down the lower limit of the T/P retrieval. Retrieving T/P to a lower altitude will further reduce our dependence on the NCEP[*] temperature data.

7. *Robust Error Estimates:* Amend our error estimates by including predetermined random error values.

8. *Long-Term Trend Reliability Studies:* Create procedures, scripts, and software to routinely monitor and describe instrument stability. Items like gas-cell content, pointing performance, and optical and spectral responses are the parameters of most interest.

9. *Data Validation:* Continue to validate and document the HALOE results by data reviews and comparisons to correlative measurements keeping the HALOE Science Team informed of the progress.

Accomplishments

During the third and final year of the contract, we made advances in extending the HALOE measurements into the upper troposphere. Our retrievals of water now extend well below the previous limits of the V19 water retrievals that relied exclusively on the H_2O radiometer channel. We further improved the differential water technique that provides for aerosol insensitive retrievals of water into the troposphere. Our cloud and related aerosol research has found that clouds near the tropical tropopause can be composed of nitric acid trihydrate (NAT) and liquid ternary aerosols (LTA). An unexpected bi-product of this study allowed us to apply our cloud/aerosol modeling to show that the spectral characteristics of polar mesospheric clouds match water ice. We have increased the accuracy of CH_4 retrievals by improving a line mixing model.

1. *Pointer-tracker:* This work was performed in the first year of the contract with the unfortunate conclusion that the gimble angle resolution was not adequate for

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[*] National Center for Environmental Prediction, formerly National Meteorological Center

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improving the temperature retrieval. However, the study led to critical requirements for future instruments, such as the Canadian occultation interferometer, ACE (http://www.ace.uwaterloo.ca), and a proposed occultation instrument for SMEX, now in the down-select phase. This will lead to high quality temperature retrievals under conditions of substantial aerosol loading, by inferring a refraction profile from image edge tracking.

2. Cloud/Aerosol Identification and Characterization:

2.1 Review of Previous Results

We have already presented a robust method for identifying cirrus cloud tops in the HALOE profiles. The V20 algorithm will make use of this procedure. Our recent discovery of tropical NAT layers in the HALOE measurements (see below) has led us to supplement the pure cirrus detection approach with a screening for NAT as well. Also, because of the increased importance of knowing the tropopause location, we reviewed the V19 tropopause identification algorithm and found that some modification was necessary.

2.2 Observations of Nitric Acid Clouds Near the Tropical Tropopause

The presence of nitric acid clouds near the tropical tropopause was proposed over a decade ago [*Hamill and Fiocco,* 1988], although little has been learned about them since. Multi-wavelength particle extinction measurements from HALOE offer the first observational evidence for the existence of tropical nitric acid clouds (TNCs) [*Hervig,* 2001]. This finding was based on spectral identification using model predictions of the HALOE response to clouds composed of ice (cirrus), nitric acid trihydrate (NAT), and liquid ternary H_2SO_4-H_2O-HNO_3 aerosols (LTA). These clouds were found to exist primarily as NAT, at latitudes between 25°S and 25°N.

The HALOE extinctions $\beta(\lambda)$ due to ice, NAT, and LTA were modeled using Mie theory with appropriate particle size distributions and refractive indices. Cirrus extinctions were calculated using ice refractive indices from *Toon et al.* [1994] and unimodal lognormal size distributions with median radii from 0.1 to 10 μm and widths from 1.1 to 3 (effective radii, R_e from 0.1 to 100 μm). Particle sizes included in these distributions encompass the range of cirrus particle sizes indicated by *Jensen et al.* [1994]. Because little is known about the physical properties of TNCs, their characteristics were estimated using nitric acid polar stratospheric clouds (PSCs) as a plausible analog. TNC size distributions were estimated from a long-term record of in situ PSC measurements over McMurdo Station, Antarctica [e.g., *Deshler et al.,* 1994]. NAT refractive indices at 196 K were taken from *Toon et al.* [1994], and LTA refractive indices were determined as a function of particle composition according to *Hervig et al.* [1997]. Background aerosols at the altitudes of interest are generally sulfate droplets and the signature from these particles was also considered. The modeled extinctions show spectral differences that are demonstrated using extinction ratios in Figure 1. Despite

some overlap, the model ratios lie in essentially distinct regions that can be used to suggest particle type through comparisons with HALOE measurements. Examples of ice and NAT detected by HALOE are shown in Figure 2.
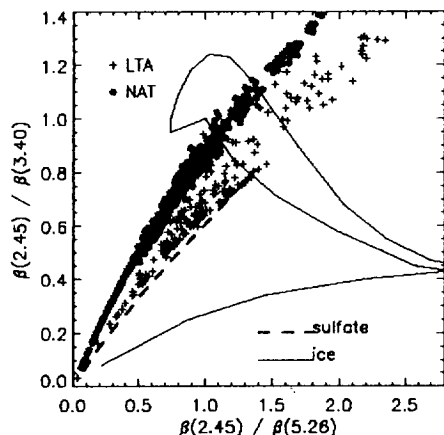

Figure 1: Extinction ratios calculated for sulfate aerosols and clouds composed of ice, NAT, and LTA. Ice results are bounded by the polygon for $\beta(2.45)/\beta(3.40) > 0.4$, and compact enough to be represented by a single curve for $\beta(2.45)/\beta(3.40) < 0.4$.

Because direct evidence of nitric acid clouds near the tropical tropopause has been lacking, the assumption has persisted that all upper tropospheric clouds are composed of ice crystals. It is well known that upper tropospheric clouds (i.e., cirrus) impact the radiative balance of our climate system, affect upper tropospheric and stratospheric water vapor budgets [*Jensen et al.*, 1996], and lead to ozone destruction through heterogeneous chlorine activation. Satellite measurements indicate cirrus occurrence frequencies near the tropical tropopause in excess of 50% [e.g., *Wang et al.*, 1996; *Hervig and McHugh*, 1999]. While cirrus investigations using remote measurements have discriminated between ice clouds and aerosols, they have not considered other cloud types. Thus, current cirrus climatologies could erroneously exclude nitric acid clouds, and the impact of high clouds on climate and chemistry may need to be revisited.

Ice, NAT, and LTA occurrence frequencies were determined from HALOE as the ratio of clouds detected to the number of profiles examined. Zonal mean occurrence frequencies versus latitude are shown in Figure 3 for HALOE measurements between 40°S and 40°N during 1998. These results indicate that NAT and LTA are restricted to tropical latitudes, and that NAT is the most common nitric acid condensate. NAT was most frequent near the equator with a peak occurrence rate of 14%. Ice also demonstrates an equatorial peak in occurrence rate (70%), and is clearly the dominant cloud type (Figure 3b). Zonal minimum tropopause temperatures (T_{min}) from NCEP analysis during 1998 were compared to the value of T_{NAT} calculated for average tropopause conditions and 0.5 ppbv HNO_3 (Figure 3a). Zonal mean tropopause temperatures are roughly 5 K higher than T_{min}. Tropopause temperatures (T_{min}) decrease sharply within the tropics (Figure 3a), and are below T_{NAT} over the same latitude range where HALOE indicates the presence of NAT. While not a strict validation, this agreement lends confidence to the HALOE NAT measurements. The methods demonstrated here are being used to identify cloud types using HALOE data. While these results have important geophysical implications, they are also important for accurate retrievals of HALOE gas measurements

near the tropical tropopause. Accurate separation of aerosol contamination requires knowledge of the particle type since this will ultimately determine the wavelength dependence of extinction. Continued investigations will explore in detail the spatial patterns of TNC occurrence, physical properties of TNC particles, and correlations between TNCs and atmospheric conditions. This work was presented at the American Geophysical Union Spring Meeting [*Hervig*, 2001], and was submitted to Geophysical Research Letters [*Hervig and McHugh*, 2001].
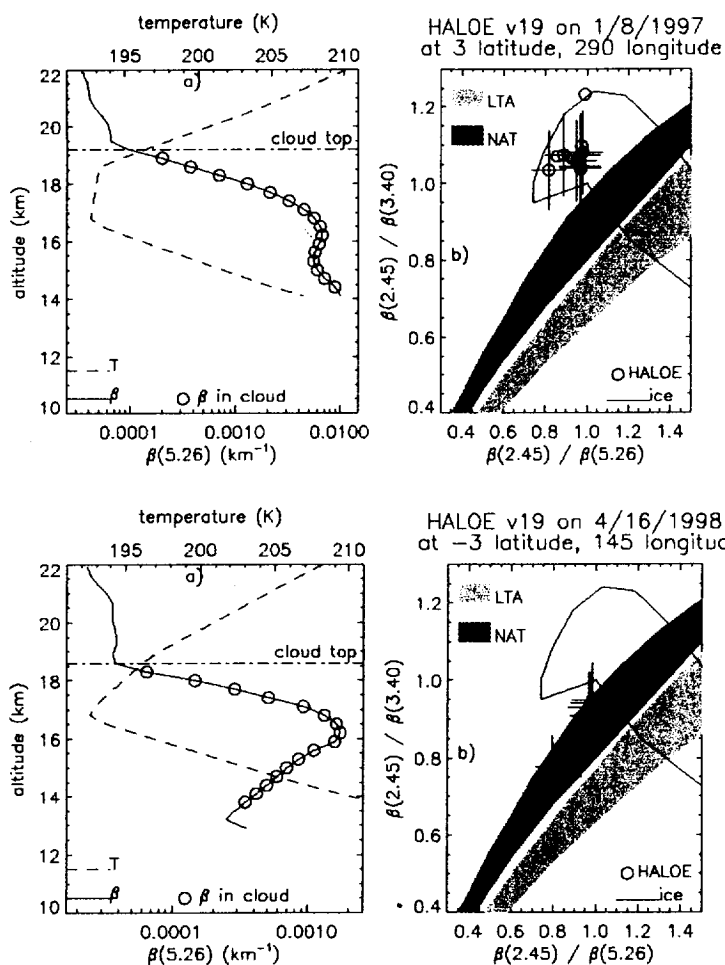

Figure 2a-b: Examples of HALOE cloud measurements near the equator that were consistent with ice (top) and NAT (lower). Symbols indicate HALOE measurements below cloud top where the ratio $\beta(3.46)/\beta(3.40)$ was within 20% of unity. a) Profiles of HALOE extinction and NCEP temperatures. Cloud tops are indicated. b) HALOE extinction ratios compared to model predictions for ice, NAT, and LTA. Error bars are shown on every other HALOE extinction ratio.
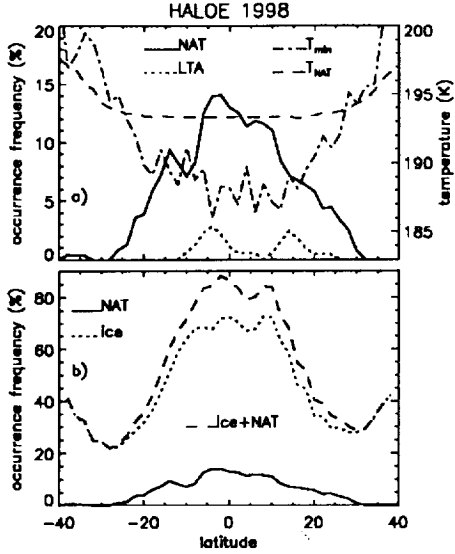
Figure 3: Cloud properties derived from HALOE measurements during 1998 at latitudes from 40°S to 40°N. a) Zonal mean occurrence frequency versus latitude for NAT and LTA. Also shown are zonal minimum tropopause temperatures taken from the NCEP analysis during 1998, and T_{NAT} calculated for average tropopause conditions and 0.5 ppbv HNO_3. b) Zonal mean occurrence frequency versus latitude for ice, NAT, and the sum of ice and NAT.

2.3 Tropopause location

The V19 (operational) algorithm identifies tropopause height (z_{trop}) as the lowest point where the estimated lapse rate ($-dT/dz$) is less than 2 K/km. The lapse rate is estimated by the least-mean-square (LMS) slope of the temperatures over eight 0.3 km layers and is assigned to the lowest of the eight layers. This was intended to reduce the effect of noise in the individual samples. However, for altitudes below 32 km, the HALOE temperature data are not retrieved but are from the National Center for Environmental Prediction (NCEP) analysis. These data have an inherent vertical resolution of about 2 km, resampled onto the 0.3 km grid. Because of this, there is negligible sample noise on the individual 0.3 km points, so the averaging of eight points is unnecessary. Also, using the bottom of an eight-layer window to estimate the lapse rate introduces a slight bias, as can be illustrated with the following hypothetical case. Consider an ideal "<" shaped temperature profile, with constant but opposite lapse rates below and above the tropopause. The gradient estimated by the LMS fit in a window will drop below the 2 K/km threshold when the bottom of the window is still a number of points below the tropopause. This clearly shows the nature of the bias in the algorithm.

To remove this bias, we simply estimate the lapse rate from the two-point temperature difference between adjacent layers. Again, z_{trop} is declared when, moving up from the bottom of the profile, the lapse rate falls below 2 K/km, with the proviso that it remains so for at least another 2 km. Results from the new two-point tropopause algorithm and V19 are compared in Figures 4 and 5. V19 values of z_{trop} are typically about 1 km lower than the new z_{trop}, and on rare occasions more than 5 km too low. These differences are significant, so the new two-point tropopause algorithm was adopted for this work and will be incorporated into V20. These improvements can be critical to algorithmic logic for retrieving water mixing ratios near the tropopause. Other more elaborate definitions of the tropopause based on potential vorticity are commonly used,

but the definition used here based on static stability is simple and adequate for the purpose of assisting in cloud detection and tropospheric retrievals.
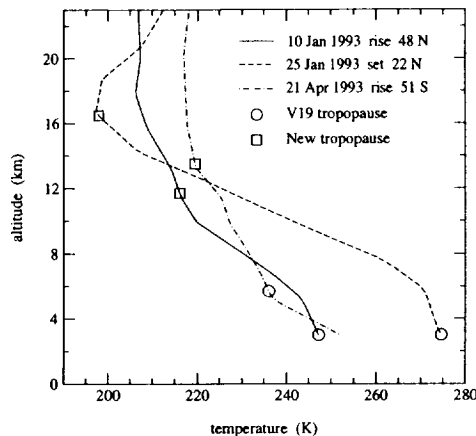

Figure 4: Examples of extreme problems with V19 tropopause locator. The V19 tropopause heights are in obvious error, while the V20 algorithm gives more reasonable results. Such extreme cases, although serious, are very rare, as detailed in Fig. 5.
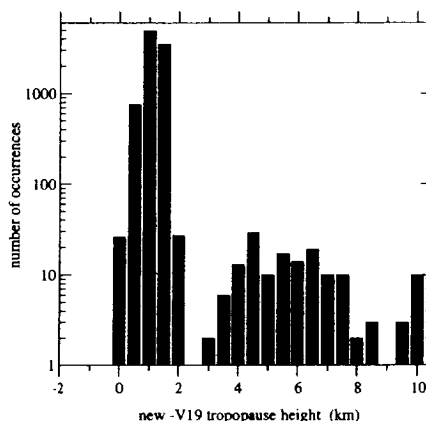

Figure 5: Distribution of modifications to the HALOE V19 tropopause heights. Data is from 1993 (9356 profiles). The new z_{trop} is on average about 1 km higher than V19. Note the log scale, which allows a clear display of the rare cases that have large (>3 km) differences to be resolved.

2.4 Polar Mesospheric Clouds

Although our work was aimed at improving HALOE tropospheric cloud measurements, our improvements suggested the potential of refined analyses of polar mesospheric clouds (PMCs). These are high latitude and high altitude clouds (~82-84km) that occur in both hemispheres near the summer solstice [*M. Alpers et al.*, 2000]. The composition of these clouds has long been assumed to be water ice [*Wegener*, 1912], but

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previous measurements have all been done at ultraviolet to near-infrared wavelengths where there is not enough information to prove this assumption. The HALOE infrared channel band passes provided a unique opportunity to overcome this obstacle. We reviewed the HALOE V19 water retrievals in the solstice time period looking for sharp changes in the water profiles near the mesopause. We assembled a list of days and events in which the changes in the water profiles indicated a PMC. We then reprocessed the level 1 product without signal smoothing and repeated the retrievals. The water product again was used to help locate sharp but very small increases in signals. An example of the HALOE signals, in units of optical depth, is shown in Figure 6 where a. PMC signature is clearly visible at 83 km. We analyzed 16 such events, averaged the results, and converted the data to extinction. The HALOE PMC extinctions are compared to model ice spectra considering PMC conditions in Figure 7. The wavelength dependence of the HALOE measurements matches closely the theoretical spectral signature of water ice. Therefore, we have spectrally observed for the first time that PMCs are composed of water ice. In addition, a first order fit to the HALOE PMC extinctions suggests cloud particle effective radii between 69 and 128 nm. These results were recently published in Geophysical Research Letters [*Hervig, et al.*, 2001]. We have since analyzed additional HALOE measurements in which we used center-sun observations to reduce the signal jitter that results from moving on the solar limb darkening curve. The results (not shown) were nearly identical.
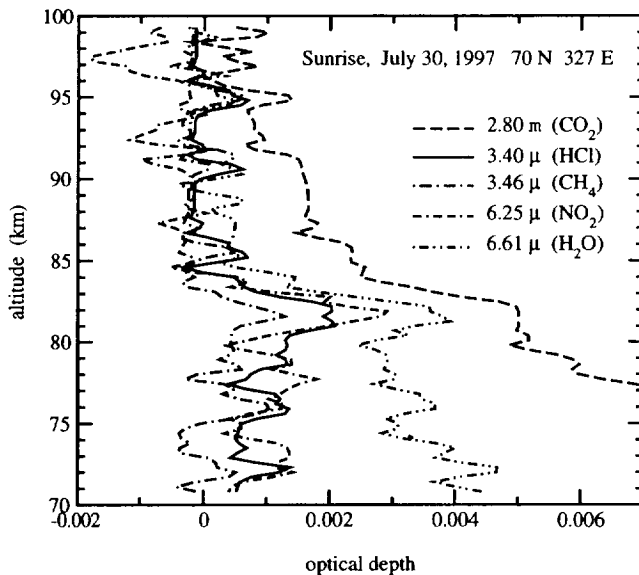

optical depth

Figure 6: HALOE optical depth profiles from sunrise on July 30, 1997, at 70° N, 327° E, without the smoothing done in production data processing. A PMC signature at ~83 km is evident as a sharp increase in optical depth. CO_2 absorption in the 2.80 µm channel, and the H_2O absorption in the 6.62 µm channel are evident as gradual increases in optical depth. The 2.45 µm, 5.26 µm, and 9.87µm channels are omitted for visual clarity.
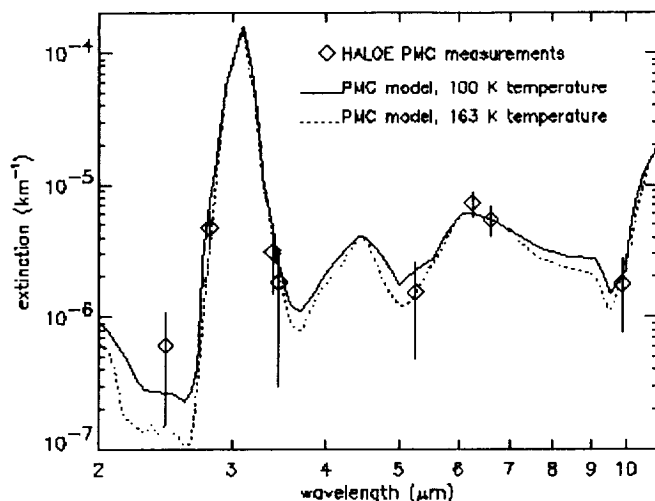
Figure 7: HALOE PMC extinctions compared to modeled extinction spectra. The HALOE data are averages based on 16 PMC measurements from July 25 to August 4, 1997, between 62°N and 72°N latitude. Vertical bars on each HALOE point represent the standard deviation of these measurements. Model spectra were calculated using the average PMC size distribution from *von Cossart et al.* [1999] with ice refractive indices for 100 K [*Bertie et al.*, 1969] and 163 K [*Toon et al.*, 1994] temperature. The model spectra were scaled to match the HALOE extinction at 6.62 μm. These scale factors were 0.76 and 0.65 for results based on the *Bertie et al.* and *Toon et al.* indices.

3. Multi-channel Retrieval

Background

HALOE was designed to probe the stratosphere. To extend retrievals of some species below this primary altitude range, we have employed new signal formulations that make full use of both band model [*Marshall, et al*, 1994] and line-by-line model [*Gordley, et al.*, 1994] capabilities. Using these new techniques, we have pushed the limits of some HALOE data products into the troposphere (with the unexpected bi-product of improved mesospheric analyses).

Extending H₂O retrievals into the upper troposphere

In a previous yearly report we discussed improvements to the broadband H_2O V retrieval. These improvements resulted from our use of a variable constraint algorithm to permit the water retrieval to more accurately resolve the rapid increase in water that begins at the hygropause. We also improved the O_2 continuum model by using the new model from *Thibault* [1997]. With these improvements we obtained a very accurate H_2O profile down to 200 mb. Below this altitude (~14 km), however, the H_2O V channel becomes nearly opaque and other techniques had to be explored to extend the water retrievals into the troposphere.

The primary goal and greatest challenge of this past year's work has been the retrieval of water in the upper troposphere. The difficulty in retrieving water at these low altitudes comes from several areas. First, water rapidly increases by two orders of magnitude from the stratosphere into the troposphere. A single HALOE channel cannot cover the entire dynamic range. Secondly, the radiometer channels that might be useful in obtaining water require an aerosol profile as an interferrent using an extrapolation of the NO aerosol retrieval to other wavelengths. This model may not be accurate enough, particularly in the presence of thin cirrus. Also, the low altitude NO aerosol retrieval requires an H_2O profile as an interferrent, and the lower portion of the NO aerosol retrieval occurs below where the H_2O V retrieval terminates. Finally, many of the radiometer channels that could be used for the retrieval of H_2O in the troposphere also need CH_4 as a known interferrent. As described later, our CH_4 tropospheric model is a constant 1.7 ppmv estimate.

To solve these problems, we decided to make use of the HF DV/V signal formulation. This signal ratio has several advantages over other techniques. First, in the troposphere, HF is essentially non-existent and no longer contributes to the DV signal, which becomes dominated by water. Thus, we switch from a HF retrieval to a H_2O retrieval. The only other significant molecular absorber is CH_4, but in the troposphere, the H_2O contribution to the DV/V signal becomes quite large as the H_2O rapidly increases and dominates the signal. Also, the DV/V formulation is nearly independent of the continuum-like aerosol absorption.

We began testing this technique and discovered that many events, most near the equator, were contaminated by clouds. While the DV/V signal is insensitive to thin cirrus, thicker clouds are a different matter, and, as was pointed out in last year's report, there is a good chance that tropospheric signals near the equator will contain absorption due to clouds. To eliminate the cloud problem, we screened the data for clouds using the HF V transmission. This channel has very little atmospheric absorption above clouds, and a cloud will cause the V signal to decrease quickly making detection relatively simple. It is also possible that a rapidly increasing water mixing ratio could also induce an absorption that looks similar to a cloud. Determining if the HF transmission is indicating a cloud or high water is not straightforward. Because we are not including these extreme water gradient events, the results may have a slightly dry bias. More study would be needed to evaluate the effect.

Our preliminary results looked very encouraging, and the obvious first step was to validate these new profiles using correlative measurements. While we have validated the V19 stratospheric H_2O measurements, the validation of tropospheric H_2O is more difficult. Every HALOE occultation has stratospheric H_2O retrievals using the H_2O V, and hence finding a coincidence with a correlative measurement is not difficult. Because we are using only HALOE measurements free of cloud contamination, the number of events that are processed is much smaller. Since tropospheric water measurements are generally ground-based, finding a good coincidence with a correlative measurement is much harder. Figure 8a illustrates this point, showing comparisons between HALOE and frost-point hygrometer measurements. [*Oltmans, et al.*, 2000]. In the first frame, the

HALOE measurement was very close in location to the Oltmans' data; it is separated by approximately three hours in time, a few tenths of degrees in latitude, and 5 degrees in longitude. Above 10 km error bars on the HALOE DV/V retrieval are very large. Below 10 km the differences in the two profiles can easily be explained by the dynamics of the lower atmosphere: large changes in water vapor occur very quickly and over short geographical distances. Figure 8b is another comparison between HALOE and frost-point hygrometer measurements and the differences are rather large. However, looking at the distance between the two measurements, it is not unexpected that the two mixing ratio profiles are quite different.

HALOE HF DV/V water 03-DEC-1998 14:24:51 Lat = 39.7 Lon = 250.4 RISE 18
H₂O Oltmans Frost Point Balloon - Boulder 03-DEC-1998 17:27:55 Lat = 40.0 Lon = 255.0 0
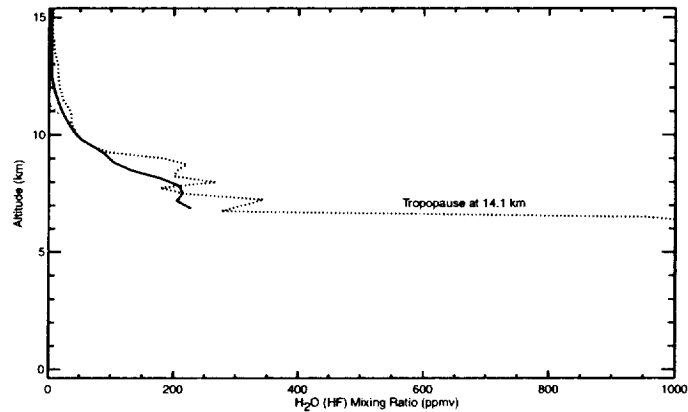
HALOE COMPARED TO OLTMANS

HALOE HF DV/V water 24-OCT-1996 13:27:34 Lat = 37.2 Lon = 252.9 RISE 18
H₂O Oltmans Frost Point Balloon - Boulder 24-OCT-1996 17:39:52 Lat = 40.0 Lon = 255.0 0
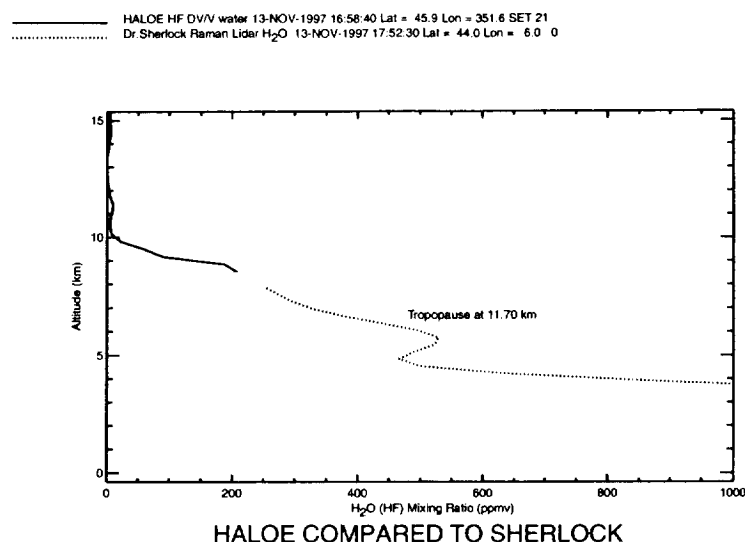

HALOE COMPARED TO OLTMANS

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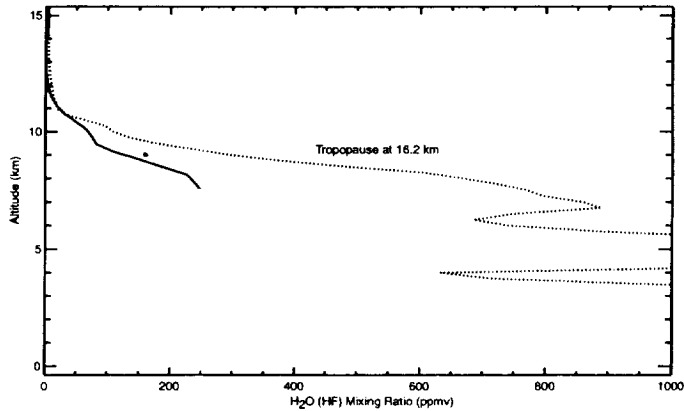
HALOE COMPARED TO SHERLOCK

Figure 8a-c: Figures (a) and (b) show comparisons of HALOE to Oltmans. Figure (c) shows a comparison to Sherlock data.

The final comparison given in Figure 8c is with lidar measurements from *Sherlock, et.al.* [1999]. To better match the lidar profile to HALOE, we have smoothed the lidar profile in altitude to match the HALOE FOV.

While the HALOE H_2O V retrieval and the HF DV/V H_2O retrievals are excellent, they do not necessarily overlap in altitude at high latitudes. In general, there will be a gap of a few km between the lower limits of the H_2O V retrievals (~14 km) and the upper limits of the of the HF DV/V retrieval (~1 km below tropopause). Since a continuous water profile is the goal, we investigated ways to bridge this gap, or merge the two profiles. As a first attempt at merging, we simply use the H_2O V down to where it is valid, (i.e., does not exceed 10 ppmv), and then switch to the HF DV/V profile once the HF DV/V retrieval is greater than 20 ppmv. An example of this merging is shown in Figure 9. Note that the gap between the two retrievals is filled in using a linear interpolation. Also, note that above ~15km where the HF DV/V retrieval starts, that the HF DV/V water profile is identical to the H_2O V mixing ratio profile; this is because the H_2O V profile is used above the starting altitude of the DV/V retrieval to help stabilize the start of the retrieval.

There are a few additional steps in the retrieval suite that could potentially improve the merged water product. We could obtain a tropospheric aerosol extinction from the HF V channel and then use the aerosol model to extrapolate the extinction to the NO V channel. The NO V channel could then be used to retrieve water. This water vapor profile would fill in the altitude gap between the H_2O V retrieval and the HF DV/V retrieval. While preliminary studies on this technique were undertaken in this year's investigations, we were unable to obtain accurate results. Recent findings, however, indicate that the V19 aerosol model may have an error in the wavelength extrapolation

function (see following section). Until this can be resolved, we will use the two channel (H_2O V and HF DV/V) results connected by linear interpolation.
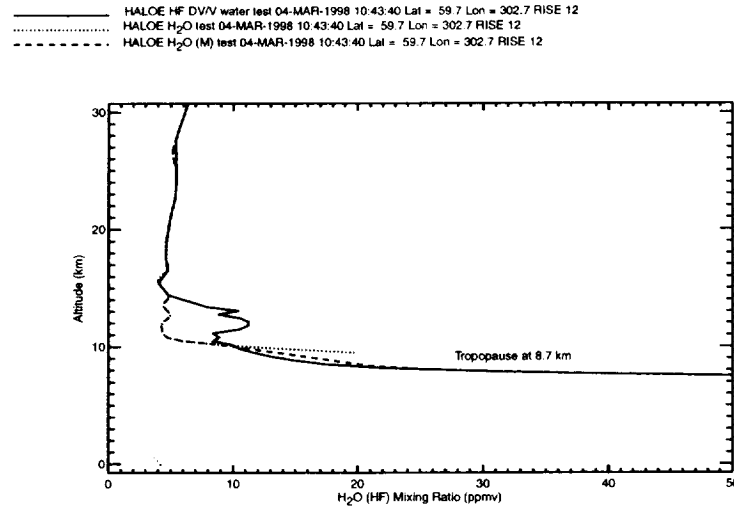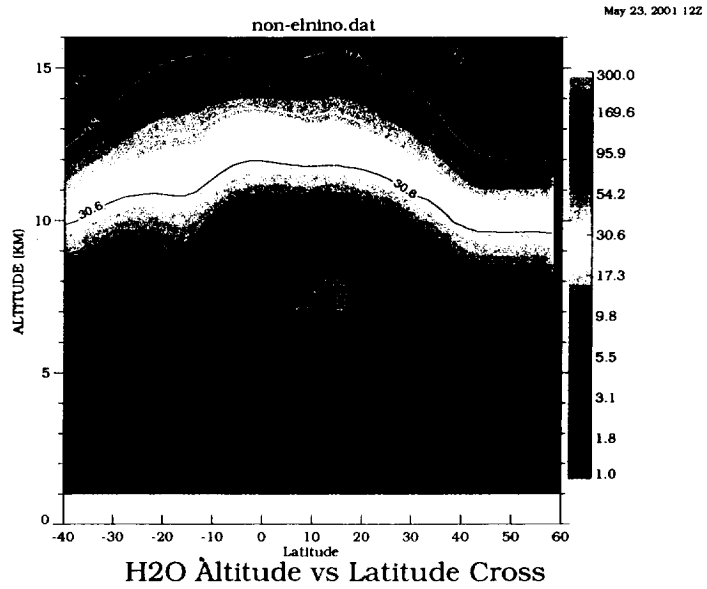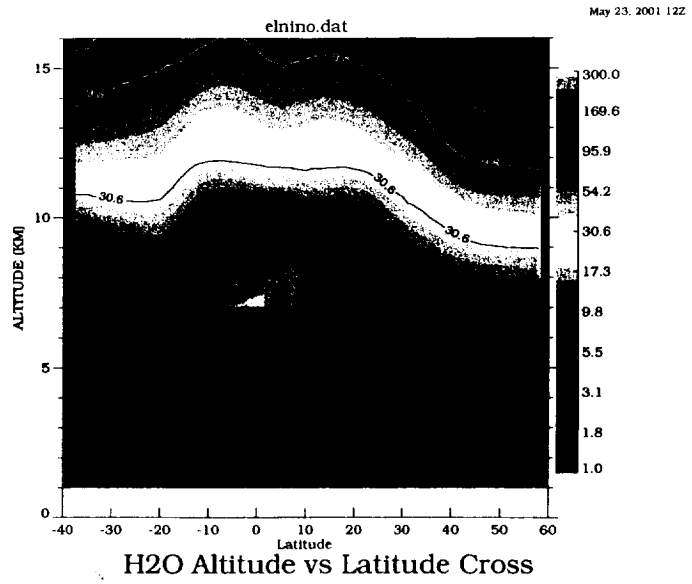

HALOE HF DV/V water test 04-MAR-1998 10:43:40 Lat = 59.7 Lon = 302.7 RISE 12
HALOE H_2O test 04-MAR-1998 10:43:40 Lat = 59.7 Lon = 302.7 RISE 12
HALOE H_2O (M) test 04-MAR-1998 10:43:40 Lat = 59.7 Lon = 302.7 RISE 12

Figure 9: Comparison of H_2O V profile (dotted), HF DV/V water profile (solid), and merged water product (dashed).

Using the merging method described above, we processed several latitude sweeps using events that were considered free of clouds. Time periods that cover both El Nino and non El Nino events were chosen as a test of the new HF DV/V water product. We then separately combined all El Nino and then all non El Nino data. Latitudinal cross section plots of these two data sets are shown in Figures 10a-b. In Figure 10c, we plotted the differences of the averaged sweeps. We presented comparisons of this type as well as comparisons to the Oltmans and Sherlock data at the SPARC meeting in Argentina in November of 2000.

In summary, software is ready for extending the HALOE water product well into the troposphere that provides excellent results. Based on this research, we now believe the DV/V can be used up to most low altitude tropopause heights (<12 km). While there is an some uncertainty in water mixing ratio for measurements that occur below the ~200 mb lower limit of the H_2O V retrieval and above where the HF ΔV/V H_2O retrieval starts, this only happens at mid to high latitudes and typically encompasses only 3-4 kilometers (less than the resolution of alternative data sets) of the lower stratosphere. Extrapolating through that region appears to provide statistically excellent results (figure 10). In addition, it has no effect on tropical and subtropical results where the tropopause is typically at or above the 200 mb level. We now have the ability to routinely measure upper troposphere water concentration.
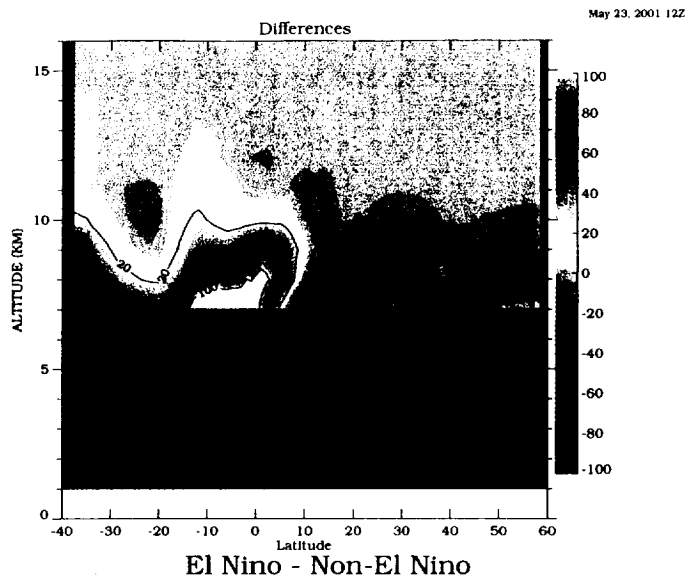
elnino.dat

May 23, 2001 12Z

H2O Altitude vs Latitude Cross

non-elnino.dat

May 23, 2001 12Z

H2O Àltitude vs Latitude Cross

May 23. 2001 12Z

Differences

El Nino - Non-El Nino

Figure 10a-c: Latitude cross sections of HALOE HF DV/V water retrievals for a) El Nino conditions, b) non El-Nino conditions and c) the differences between El Nino and non-El Nino conditions.

Improving low altitude CH₄ retrievals

The current CH_4 DV/V retrievals stop near 150 mb because of near saturation of the gas correlation difference signal DV. We attempted to extend the CH_4 retrievals downward using other channels and new signal formulations such as the broadband HCl channel which is dominated by methane absorption. Our initial investigations used the CH_4 V and HCl V signals, which unlike the DV/V retrieval are sensitive to aerosol as an interfering absorber. To retrieve methane using the CH_4 V and HCl V measurements, the aerosol was estimated (as opposed to retrieved) from the NO channel aerosol using a Mie scattering sulfate model. These retrievals resulted in CH_4 profiles that were biased from the DV/V retrievals as shown in Figure 11. In addition, the HCl and CH_4 V retrievals were themselves biased from each other. After an exhaustive study of potential errors in the aerosol model and various multi-channel approaches to avoid such problems, it was determined that the inconsistency in CH_4 retrievals using the HCl V and CH_4 V channels during light aerosol conditions was due to a deficiency in the NO_2 line parameters in the HCl channel band pass. This has now been corrected for the version 20 algorithm. Although this has brought the CH_4 V and HCl V retrievals into much closer agreement, they are still inconsistent with the CH_4 DV/V (gas correlation) methane retrievals, being about 15-20% lower than the gas correlation results. Also, the DV/V and V retrieval show agreement in the rare condition of nearly aerosol free air (ex. above 25 km and in the polar vortex after PSCs have melted). In addition, the gas correlation results show excellent agreement with correlative measurements. This tends to indicate a problem with the aerosol model. We were unable to resolve the discrepancy, so we chose to use the gas correlation results extrapolated to and merged with a tropospheric constant value of 1.7 ppmv for use in the gas correlation water retrieval, which has only a slight dependence on methane interference. An example of this combined CH_4 model is shown

in Figure 12. Note that the gas correlation retrieval (solid line) was run at high resolution, as discussed later in section 5.
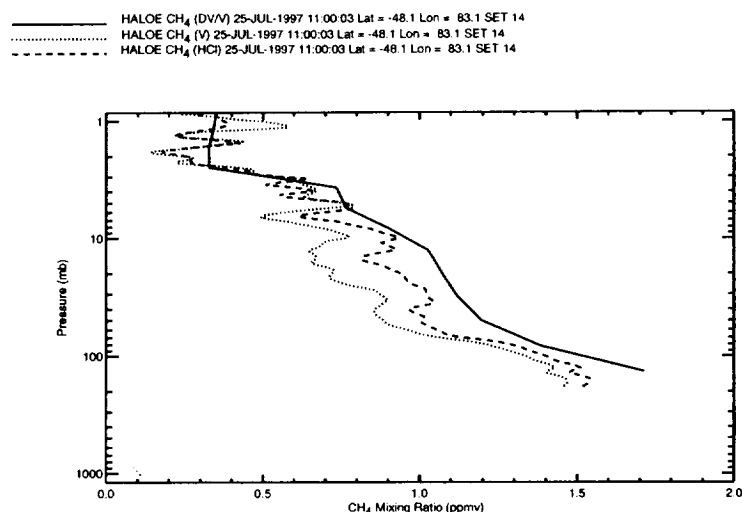

Figure 11: Comparison of CH₄ retrieved using DV/V (solid), CH₄ V (dotted) and HCl V (dashed) before NO₂ correction. The correction of NO₂ line parameters in the HCl V channel now brings it into agreement with the CH₄ V channel results.
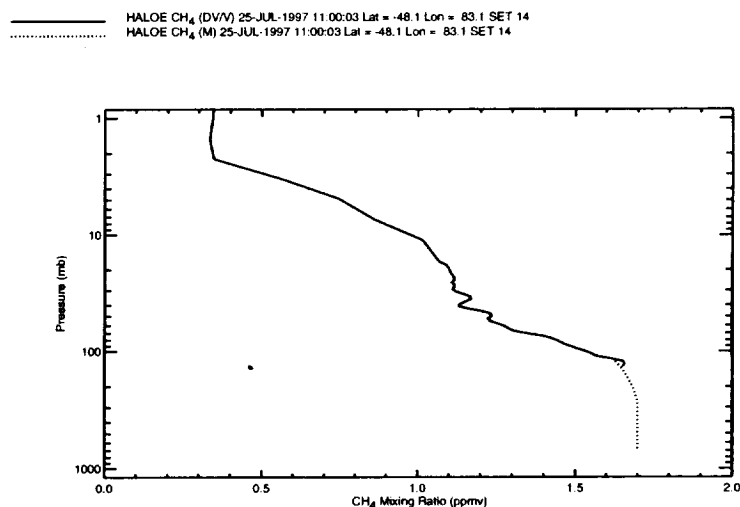

Figure 12: The solid line is the CH₄ DV/V retrieval and the dotted is this profile rolled off to 1.7 ppmv in the troposphere.

In addition to an error in the 3.40 μm HCl channel aerosol retrieval due to the same NO₂ line deficiency as in the case of the CH₄ retrieval, we have discovered that the aerosol spectral model is inconsistent with HALOE aerosol data in periods of low aerosol

loading. This is a problem that must be resolved if low altitude (<15 km) methane is to be inferred from HALOE data. However, the positive result is that the HALOE data reliably indicates that the accepted model for stratospheric aerosol indices of refraction is not accurate in conditions of low aerosol concentration (i.e. near background condition). Therefore, the HALOE data could be used to greatly improve the sulfate aerosol model, a potentially valuable contribution to stratospheric research. Once in hand, the model could be used to allow methane retrievals into the upper troposphere by modeling the aerosol extinction in the methane V signal as a function of aerosol extinction in the nitric oxide channel.

Correction of PMC effects

Current V19 HALOE water vapor data near the mesopause are corrupt whenever PMCs appear in the line-of-sight. Previously, we had developed a "differential" retrieval for water vapor that used both the 6.26 and 6.61 μm channels to remove the effect of contaminant absorption by particulates in the troposphere. As discussed above, we have recently confirmed that PMC's are composed of water ice particles [*Hervig et al.* 2001]. Using this differential information, we were able to develop a more rigorous retrieval formulation that accurately models the PMC particulate extinction in the both the 6.61 and 2.80 μm channels, removing the largest error source from both the mesospheric water and temperature retrievals.

In this new technique we iteratively retrieve three quantities: 1) PMC extinction from the 6.26 μm channel, 2) temperature from the 2.80 μm channel and 3) water vapor from the 6.62 μm channel. Water vapor, carbon dioxide and PMC particles dominate the extinctions in these three wavebands above 70 km. In the water and temperature retrievals we model the PMC extinction by extrapolating the extinction retrieved at 6.26 μm. The extrapolation assumes a wavelength dependence calculated from Mie scattering by small ice particles. *Hervig, et al.* [2001] confirmed this spectrum experimentally.

In production processing, V19 retrievals first smooth the transmission signals in altitude to improve signal-to-noise. Because we expect PMC layers to be relatively thin (1-3 km), we are forced to omit this smoothing in the PMC correction process. Unfortunately, the transmission signals at these altitudes are very small, and because the 6.26 μm channel has relatively high noise, other means of noise reduction are needed. We achieve this by using daily average transmission signals. (There are nominally 15 occultations per day, in a narrow latitude band). Other methods for improving signal-to-noise are being investigated, but this approach is wholly adequate for producing robust daily mean water vapor and temperature measurements, even in the presence of PMCs. Figures 13 and 14 illustrate the effect of the PMC correction.
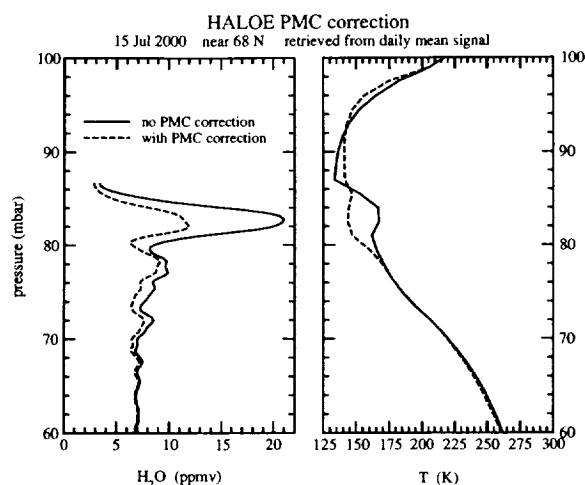
Figure 13: PMC correction to the water and temperature retrievals for HALOE sunrise on July 15, 2000, near 68 N. The dashed lines indicate the V19 algorithm, and the dashed are the retrievals using the new PMC model in which the extinction is retrieved in the 6.26 μm channel and extrapolated to the 6.61 and 2.80 μm channels (water and CO_2 respectively) using an ice model. Note the dramatic reduction in water vapor at the PMC altitude of 83 km. The corrected temperatures dip below 150 K at this altitude, thought to be the temperature required for PMC formation. These retrievals were done on the daily (zonal) mean signals.
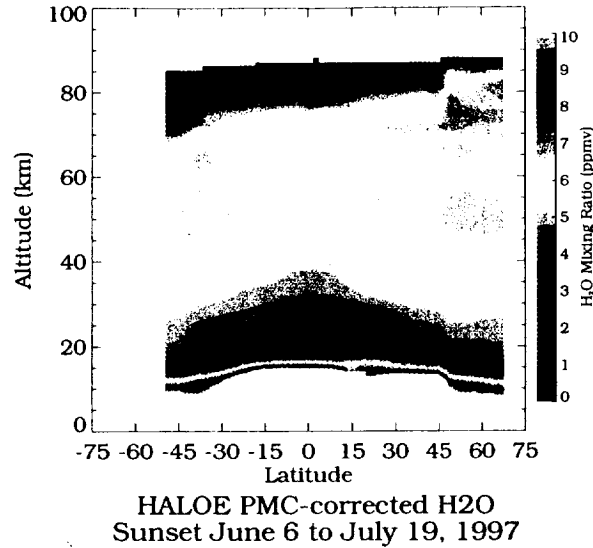

HALOE V19 H2O
Sunset June 6 to July 19, 1997

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HALOE PMC-corrected H2O
Sunset June 6 to July 19, 1997
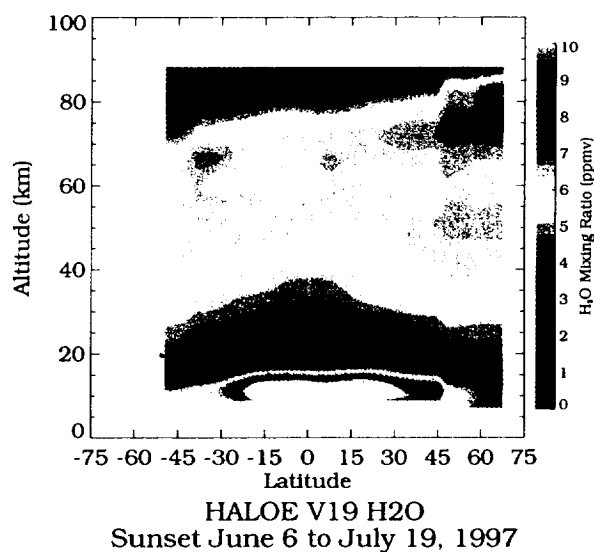
Figure 14: PMC correction to HALOE water vapor data. a) Data from the V19 algorithm show a large (incorrect) feature of high water vapor in the vicinity of PMCs. b) PMC corrected water vapor. With the PMC contamination removed, good measurements of the water vapor content in the polar mesopause are now available. To achieve the necessary signal-to-noise, the retrievals shown in these latitude cross-sections are from daily (zonal) mean signals.

Section 3 Summary

In summary, we used the HF DV/V signal formulation to obtain excellent tropospheric water measurements. We merge this water profile with the H_2O radiometer retrieval to form a continuous water product that can be used in both research and further retrieval improvements. While we were unable to retrieve CH_4 in the upper troposphere, we were able to improve our tropospheric CH_4 profiles for algorithm use by using high resolution retrievals and transitioning the profiles to 1.7 ppmv in the troposphere. We also used the differential H_2O technique to obtain better water vapor retrievals, temperature retrievals, and PMC extinction from signals with PMC signatures. Finally, we learned that there is a deficiency in the NO_2 line parameters used in the CH_4 V aerosol retrievals and have determined that the standard model for stratospheric aerosol indices of refraction may be in error in times of low aerosol extinction.

4. *Forward Model Improvements*

For V20 we have implemented CH_4 line mixing [*Benner, et al.*, 1998], which provides a much better model of the CH_4 line shapes. To calculate the line mixing parameters, methane absorption in the methane and HCl channels is simulated using the full relaxation matrix rather than a Lorentz line profile. The two calculations are equivalent when the off diagonal elements of the relaxation matrix are all zero. However, there are about 100 of the off diagonal matrix elements in this spectral region which are large enough to be significant. For version 19, the ratio of self to air induced off diagonal

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matrix element coefficients was assumed to be the same as the ratio of the self to air Lorentz half widths and the temperature dependence was assumed to be the same as those of the corresponding Lorentz half widths. For version 20, separately measured values of the self and air induced off diagonal matrix element coefficients are used along with separately measured temperature dependence of the air induced coefficients. The temperature dependence of the self induced off diagonal relaxation matrix element coefficients are rough estimates, but they are not very important due to the small range of temperatures of the methane channel correlation cell and the very low mixing ratio of methane in the atmosphere. The imaginary part of the off diagonal relaxation matrix elements is assumed to be zero. Figure 15 shows the effects of the V19 version of the line mixing code. The effects of line mixing are important in the lower portions of the retrieval. The final version of line mixing will be used in V20.
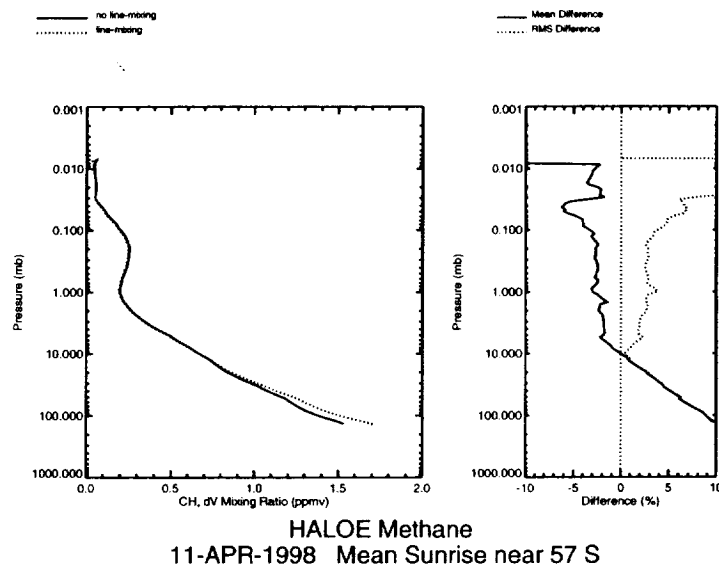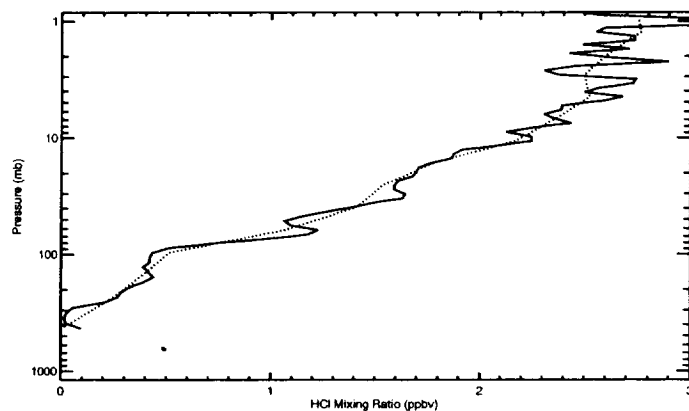

HALOE Methane
11-APR-1998   Mean Sunrise near 57 S

Figure 15: Effect of methane line mixing on the methane retrieval. Spectroscopic line parameters were determined by fitting experimental spectra with and without line mixing. This results in different line parameters even for non-mixed lines. The differences for P < 10 mb arise from these non-mixed line parameter differences. Line mixing becomes increasingly important for P > 10 mb. Similar results are seen in the HCl retrieval.

A final forward model issue concerns the HALOE O_3 retrievals. The HALOE O_3 retrievals have shown a small bias with respect to correlative measurements below the peak in the stratosphere. This bias is in part due to the use of a broadband approximation of the forward calculation in the retrievals. A simple solution is to perform the retrievals using the line-by-line code, as is done in the gas correlation channels. We suggest doing the O_3 channel retrievals using the line-by-line code with a spacing of 0.6 km in the lower altitudes where it is important and not as computationally excessive as at high altitudes.

5. *Fine Vertical Resolution Gas Channel Retrievals*

Because the retrievals of NO, CH_4, HCl, and HF (the gas correlation channels) require a line-by-line forward model as opposed to the use of a band model, these retrievals are performed on a coarser altitude grid than the radiometer channel retrievals. The use of this coarse altitude spacing (3.0 km) keeps the computational time to reasonable limits, but prohibits the resolution of fine features in the retrievals as accomplished with the radiometer channels. Because the computational speed of computers has increased dramatically since HALOE's launch, it is now feasible to reduce the layer spacing to something more commensurate with the layer spacing of the band model retrievals. Examples of gas correlation channel retrievals are shown in Figure 16. Note how the high resolution retrievals are able to resolve the finer features; the ringing in the upper portion of the HCl retrievals can be eliminated by using a variable constraint technique like that used in the H_2O retrieval -- tight constraints at high altitudes where the signal to noise is low and loose constraints at lower altitudes. Because of the obvious improvement and consistency with the other products (O_3, H_2O, NO_2 and aerosol), we recommend reprocessing using this higher resolution retrieval grid. The operational algorithm was designed to accommodate the higher resolution, should the computation resources become available.

HALOE HCl hi_res 23-SEP-1995 19:04:57 Lat = -56.0 Lon = 161.3 RISE 24
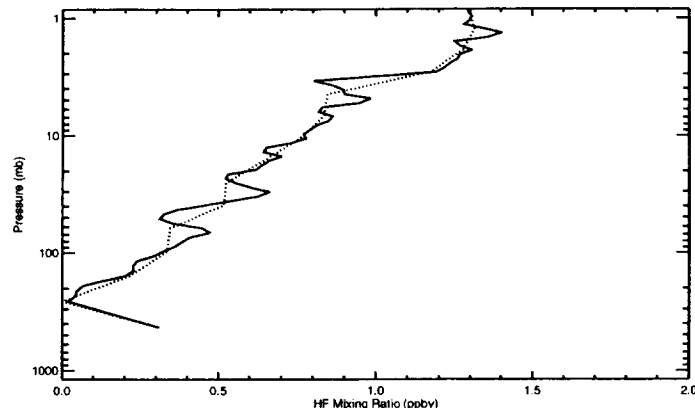HALOE HCl low_res 23-SEP-1995 19:04:57 Lat = -56.0 Lon = 161.3 RISE 24

Figure 16a-b: Line-by-line retrievals of a) HCl and b) HF showing the improvement in the retrievals that result from using a 0.3 km spacing in the retrievals (solid line). A retrieval using the V19 spacing of 3.0 km is indicated with the dotted lines.

6. *Improved Temperature-Pressure Retrieval*

As mentioned in the previous report, we now believe that retrieving temperature to lower altitudes is not feasible with the HALOE CO_2 channel band pass. Still, small improvements are possible. We tested the sensitivity of the CO_2 channel transmission signal to potential updates in the spectral line parameters of H_2O. Since the water absorption is approximately 15% of the total channel absorption at 1 mb, the expected update to the H_2O half widths should be included in any future reprocessing of HALOE data. There was also a concern that the weak HNO_3 band in the CO_2 channel band pass might be strong enough that we should include it in the channel transmission calculations. This concern was raised due to the availability of new spectral line parameters for HNO_3. We determined that the absorption of HNO_3 in the CO_2 channel is still very small and can be ignored.

7. *Error Estimates*

As mentioned in last year's report, the error estimate work is being performed through other avenues and the results will be discussed in a separate report.

8. *Long-Term Trend Analyses*

This was addressed in the first year of the task. No additional work was undertaken.

9. *Data Validation*

Validation of new HALOE data has been ongoing in which we reviewed all the HALOE products looking for events that contained profiles that were questionable. Only a few profiles were of concern. We also needed to compare the new tropospheric water retrievals to correlative measurements. As mentioned in section 3, the new water products require correlative measurements in the troposphere, causing the availability of close coincidences free of clouds to be a major problem. As discussed in last year's' report, sources of correlative measurements include the MOZAIC aircraft measurements [*Marenco et al.*, 1998], lidar measurements such as those by *Browell et al.* [1996], Raman lidar measurements at the Arm site in Oklahoma and Haute Province, and, sources through our involvement in SPARC [*Kley, et.al.* 2000]; we obviously have a substantial reservoir of measurements that can be used in our comparisons.

Over the years as part of the testing and validation process, we have assembled a thorough set of data analysis products that we rely on to diagnose and validate the data. This includes sunrise/sunset differences, comparisons to related species, and trends of HALOE parameters pertaining to instrument stability. These products would be used extensively in testing the next data version.

Proposed Reprocessing Plans

We now summarize the progress we have made in this and the previous two years efforts. Each item would need to be carefully tested and validated when reprocessing is undertaken. This will include recomparisons to correlative measurements and, in the case of the tropospheric retrievals, first time comparisons. Testing will need to be carried out on a number of sweeps to test all data conditions. From the list given below, it is clear that reprocessing the entire HALOE data set can substantially improve the HALOE data product.

- Upper Tropospheric water using HF DV/V algorithm
- H_2O V retrieval results using the new Thibault continuum and loose constraint algorithm at low altitudes to accurately characterize sharp low stratosphere features.
- Connection of the tropospheric water and stratospheric water retrievals when they do not overlap because of a low altitude tropopause (i.e. high latitude).
- High resolution gas correlation channel retrievals
- CH_4 retrievals using new line mixing software with attention to how well the retrievals merge into the tropospheric model
- Cloud/aerosol products including a vastly improved new cloud height product, and improved cloud screening for gas retrievals.
- NO_2 retrievals using new Thibault continuum
- New H_2O line parameters in the CO_2 channel
- Better tropopause altitude identification
- Low altitude ozone retrievals using a line-by-line forward model.

- Better aerosol in the 3.40 μm channel by inclusion of NO_2 as an interferrent in the HCl aerosol retrieval
- Accurate temperature and water at the summer mesopause.

A notably improved and expanded HALOE data set can be obtained by implementing these changes. Since these improvements have been implemented in software under this grant, reprocessing could proceed immediately. HALOE has proven to be one of the most successful long-term experiments onboard UARS, and could offer an even better data set for scientific investigations by implementing the proposed improvements.

Publications Resulting From This Proposal

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Goddard Space Flight Technical Monitor – Anne Douglass

14. ABSTRACT

This report details the ongoing efforts by GATS, Inc., in conjunction with Hampton University and University of Wyoming, in NASA's Mission to Planet Earth UARS Science Investigator Program entitled "HALOE Algorithm Improvements for Upper Tropospheric Sounding." The goal of this effort is to develop and implement major inversion and processing improvements that will extend HALOE measurements further into the troposphere. In particular, O_3, H_2O, and CH_4 retrievals may be extended into the middle troposphere, and NO, HCl and possibly HF into the upper troposphere. Key areas of research being carried out to accomplish this include: pointing/tracking analysis; cloud identification and modeling; simultaneous multichannel retrieval capability; forward model improvements; high vertical-resolution gas filter channel retrievals; a refined temperature retrieval; robust error analyses; long-term trend reliability studies; and data validation. The current (first year) effort concentrates on the pointer/tracker correction algorithms, cloud filtering and validation, and multichannel retrieval development. However, these areas are all highly coupled, so progress in one area benefits from and sometimes depends on work in others.

15. SUBJECT TERMS
HALOE, UARS, remote sensing

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